

# Sign Rules for Anisotropic Quantum Spin Systems

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We present new and exact “sign rules” for various spin- $s$  anisotropic spin-lattice models. It is shown that, after a simple transformation which utilizes these sign rules, the ground-state wave function of the transformed Hamiltonian is positive-definite. Using these results exact statements for various expectation values of off-diagonal operators are presented, and transitions in the behavior of these expectation values are observed at particular values of the anisotropy. Furthermore, the effects of sign rules in variational calculations and quantum Monte Carlo calculations are considered. They are illustrated by a simple variational treatment of a one-dimensional anisotropic spin model. [PACS numbers: 75.10.Jm, 02.70.Lq, 03.65.Fd, 75.50.Ee]

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Exact results for quantum many-body systems are rare. They are, therefore, always valuable as yardsticks against which numerical or semi-analytical methods may be measured. Such exact results acquire additional value when they can be used as actual input to improve one or more of the approximate methods. Such input is often useful, for example, in tailoring a trial or starting many-body wave function to preserve certain exact properties. In some instances they can even be practically essential for the successful implementation of particular techniques. An example is provided by the fixed-node quantum Monte Carlo (QMC) method, which provides a means to circumvent the infamous “minus sign problem” inherent in simulating many-fermion systems, but at the cost of requiring good (and, ideally, exact) information on the nodal surface of the many-fermion wave function. In this paper we provide several exact results of such “sign rules” (which exactly define the nodal surfaces) for some general classes of anisotropic spin-lattice models. These models are of considerable interest both in their own right and as models of real (low-dimensional) magnetic materials.

In 1955 Marshall [1] used a variational method to study the isotropic spin-half Heisenberg antiferromagnet (HAF) specified by the Hamiltonian

$$H = J \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j \quad , \quad (1)$$

where the sum on  $\langle i,j \rangle$  counts each nearest-neighbor pair once and once only, and  $J$  is positive. Furthermore, the lattice was assumed to be *bipartite* (i.e., the lattice can be divided into two sublattices ( $A,B$ ) such that all nearest neighbors of a site on one sublattice lie on the other and *vice versa*). The total number of atoms was  $N$  and the spatial dimensionality was not restricted. In the course of this paper it was proven that the exact ground-state wave function can be written as

$$|\Psi\rangle = \sum_I c_I |I\rangle \quad , \quad (2)$$

where  $\{|I\rangle\}$  are the usual basis states in the Ising representation. The coefficients  $\{c_I\}$  were proven to have the property that,

$$c_I = (-1)^{\phi(I)} a_I \quad , \quad (3)$$

where the coefficients  $\{a_I\}$  are all positive real numbers or zero and  $\phi(I)$  is the eigenvalue, with respect to the corresponding eigenstate  $|I\rangle$ , of the operator,

$$\phi = n_A \quad , \quad (4)$$

which counts all of the spin-half ‘up’ states on the  $A$ -sublattice. Lieb and Mattis [2] were able to prove that the ground state of the HAF was a singlet following the work of Marshall [1] and Lieb *et al.* [3].

Indeed, these results for the HAF model on a bipartite lattice are a consequence of a property of non-positive matrices. The Hamiltonian of Eq. (1) is transformed in the following manner,

$$H' = e^{i\pi\phi} H e^{-i\pi\phi} \quad . \quad (5)$$

It is seen that  $H'$  of Eq. (5) now contains only non-positive off-diagonal interactions with respect to the Ising basis states. Hence the ground state of the HAF corresponds to the eigenstate of largest magnitude eigenvalue which is positive-definite via the Perron–Frobenius theorem [4]. Munro [5] and Parkinson [6] were also able to extend these results to the spin-one biquadratic model on a bipartite lattice in various phases. They showed that the ground eigenstates are positive-definite and also non-degenerate. Finally, Klein [7] utilized this knowledge afforded by the Perron–Frobenius theorem for Heisenberg models to prove six theorems relating to ground-state features of these models. Amongst these theorems was one which stated that the ground-state expectation value of  $\mathbf{s}_i \cdot \mathbf{s}_j$  for these models is positive or negative depending on whether  $i$  and  $j$  are on the same or different sublattices, respectively.

In this article, we present new sign rules for various spin- $s$  anisotropic spin systems. The transformation of

Eq. (5) for these sign rules is utilized to force the off-diagonal interactions of the Hamiltonians to be always non-positive. A property of positive or negative semi-definite matrices is that the eigenvector corresponding to the eigenvalue of  $H'$  of largest magnitude (i.e., the ground-state energy here) contains only non-negative elements, and so the ground-state wave function is positive-definite.

The first model that we consider is the  $XYZ$  model, which has a Hamiltonian given by

$$H_{XYZ} = \sum_{[i,j]} \left\{ J_{i,j}^x s_i^x s_j^x + J_{i,j}^y s_i^y s_j^y + J_{i,j}^z s_i^z s_j^z \right\},$$

$$= \sum_{[i,j]} \left\{ a_{i,j} s_i^z s_j^z + b_{i,j} (s_i^+ s_j^- + s_i^- s_j^+) \right. \\ \left. + c_{i,j} (s_i^+ s_j^+ + s_i^- s_j^-) \right\}, \quad (6)$$

where  $a_{i,j} = J_{i,j}^z$ ,  $b_{i,j} = (J_{i,j}^x + J_{i,j}^y)/4$  and  $c = (J_{i,j}^x - J_{i,j}^y)/4$ . The index  $i$  in Eq. (6) runs over all  $N$  sites on a bipartite lattice and  $j$  runs over all sites which are on the opposite sublattice to  $i$ . The square bracket  $[i, j]$  indicates that each bond is counted once and once only.

The second such model that we shall consider is the single-ion anisotropy (SIA) model, given by

$$H_{SIA} = D \sum_i (s_i^x)^2 + \sum_{[i,j]} J_{i,j} \mathbf{s}_i \cdot \mathbf{s}_j,$$

$$= \sum_{[i,j]} J_{i,j} \left\{ s_i^z s_j^z + \frac{1}{2} (s_i^+ s_j^- + s_i^- s_j^+) \right\}$$

$$+ \frac{D}{4} \sum_i \left\{ (s_i^+)^2 + (s_i^-)^2 + 2(s(s+1) - (s_i^z)^2) \right\}. \quad (7)$$

Again, the index  $i$  in Eq. (7) runs over all  $N$  sites on a bipartite lattice and  $j$  runs over all sites which are on the opposite sublattice to  $i$ .

Finally, we also consider the transverse Ising model (TIM), which has a Hamiltonian given by

$$H_{TIM} = \sum_{[k_1, k_2]} \Omega_{k_1, k_2} s_{k_1}^z s_{k_2}^z + \frac{\lambda}{2} \sum_i (s_i^+ + s_i^-). \quad (8)$$

For the TIM, we place no restriction on the lattice type and  $k_1$  and  $k_2$  are allowed to run over all lattice sites with  $k_1 \neq k_2$ . Furthermore, note that adding extra diagonal terms in Eqs. (6-8) (such as an external magnetic field or crystal field anisotropy in the  $z$ -direction), or letting  $i$  and  $j$  in Eqs. (6) and (7) run over the same sublattice but, in this case, explicitly restricting  $b_{i,j} \leq 0$  in Eq. (6) and  $J_{i,j} \leq 0$  in Eq. (7), do not change the following sign rules.

We now define the following operators,

$$m_A = \sum_{l_A} s_{l_A}^z; \quad m = \sum_l s_l^z, \quad (9)$$

where  $l_A$  runs over all  $N/2$   $A$ -sublattice sites and  $l$  runs over all  $N$  sites on both sublattices. Note that for eigenstate  $|I\rangle = \bigotimes_{l=1}^N |s_l, m_l\rangle$ , where  $s_l^z |s_l, m_l\rangle = m_l |s_l, m_l\rangle$ ,  $m$  and  $m_A$  have eigenvalues denoted by  $m(I)$  and  $m_A(I)$ , respectively. Note that the following sign rules are fully defined by the form of the operator  $\phi$  which, in turn, gives the set of eigenvalues  $\{\phi(I)\}$ . Furthermore, these eigenvalues determine the signs of the  $\{c_I\}$  coefficients via Eq. (3) for the expansion of the ground-state wave functions, Eq. (2), of the anisotropic Hamiltonians of Eqs. (6-8). The sign rules are thus defined by,

$$\left. \begin{array}{ll} \phi = 1 & ; \text{ rule (A)} \\ \phi = m_A & ; \text{ rule (B)} \\ \phi = m/2 & ; \text{ rule (C)} \\ \phi = m_A + m/2 & ; \text{ rule (D)} \\ \phi = m & ; \text{ rule (E)} \end{array} \right\} \quad (10)$$

Furthermore, note that rule (B) is a reformulation, for general spin quantum number, of the Marshall-Peierls sign rule for the spin-half HAF given by Eqs. (3-4). It is found that the first four sign rules apply to the  $XYZ$  and SIA models in the following regimes,

$$\left. \begin{array}{lll} \text{Rule} & XYZ \text{ model} & \text{SIA model} \\ \text{(A)} & b_{i,j} \leq 0, c_{i,j} \leq 0 & D \leq 0, J_{i,j} \leq 0 \\ \text{(B)} & b_{i,j} > 0, c_{i,j} \geq 0 & D \leq 0, J_{i,j} > 0 \\ \text{(C)} & b_{i,j} \leq 0, c_{i,j} > 0 & D > 0, J_{i,j} \leq 0 \\ \text{(D)} & b_{i,j} > 0, c_{i,j} < 0 & D > 0, J_{i,j} > 0 \end{array} \right\} \quad (11)$$

for all values of  $i$  and  $j$  on opposite sublattices. (Note again that we do not allow the existence of any “frustrated” interactions in Eqs. (6) or (7).) For the TIM, it is found that rule (A) applies when  $\lambda \leq 0$ , and rule (E) applies when  $\lambda > 0$  for all signs and strengths of the coefficients  $\Omega_{k_1, k_2}$  of the Ising interaction in Eq. (8).

We once again note that the off-diagonal interactions of  $H'$  of Eq. (5) with respect to a complete set of Ising states are now always non-positive. Hence the ground-state eigenvector of  $H'$  contains only non-negative elements and so may be written as  $|\Psi'\rangle = \sum_I a_I |I\rangle$ , with  $a_i \geq 0 \forall I$ .

It is also possible to prove exact relations [7] (in some cases) for expectation values of various off-diagonal operators. In order to illustrate this we define an  $XXZ$  model for a bipartite lattice in which we set  $J_{i,j}^x = J_{i,j}^y$  and  $J_{i,j}^z = 1$  in Eq. (6). Hence we see from the table above that the sign rules are of type (A) for  $J_{i,j}^x \leq 0$  and of type (B) for  $J_{i,j}^x > 0$ . We define the spin-spin correlation function in the  $x$ -direction, given by

$$G^{xx}(r) = \frac{\langle \Psi | \sum_l s_l^x s_{l+r}^x | \Psi \rangle}{N \langle \Psi | \Psi \rangle}, \quad (12)$$

and the localized magnetization in the  $x$ -direction to be,

$$M^x(l) = \frac{\langle \Psi | s_l^x | \Psi \rangle}{\langle \Psi | \Psi \rangle}. \quad (13)$$

For the XXZ model with  $J_{i,j}^x > 0$ , it can be shown that if  $r$  in Eq. (12) connects sites on opposite sublattices then  $G^{xx}(r) \leq 0$  and if  $r$  connects sites on the same sublattice then  $G^{xx}(r) \geq 0$ . Similarly for  $J_{i,j}^y > 0$ , it can be shown that the sign of  $M^x(l)$  when  $l$  is a site on one particular sublattice must be the opposite to the sign of  $M^x(l)$  when  $l$  is a site on the other sublattice. For  $J_{i,j}^x < 0$ , one can show that  $G^{xx}(r) \geq 0 \forall r$  and that  $M^x(l) \geq 0 \forall l$ . For the transverse Ising model, it is found for any value of  $\lambda$  that  $G^{xx}(r) \geq 0 \forall r$ . By contrast, it is found that  $M^x(l) \leq 0 \forall l$  for  $\lambda > 0$ , and that  $M^x(l) \geq 0 \forall l$  for  $\lambda < 0$ . We note that other such relations exist for the models presented here, although they are not discussed further in this article.

In order to illustrate the usefulness of the sign rules given here, we now perform a simple variational calculation for an anisotropic spin system which utilizes some of these sign rules. The system in question is a spin-half one-dimensional model [8] in which the anisotropy is in the  $x$ -direction such that  $J_{i,j}^x \equiv -\Delta$ ,  $J_{i,j}^y = 1$ , and  $J_{i,j}^z = -1$  in Eq. (6) and  $i$  and  $j$  are always nearest neighbors. Hence, from Eq. (11) the sign rules are of type (A) for  $\Delta \geq 1$ , of type (D) for  $-1 < \Delta < 1$ , and of type (B) for  $\Delta \leq -1$ . The ground-state energy of this system using Eq. (2) may be written as,

$$E = \frac{\sum_{I_1, I_2} c_{I_1}^* c_{I_2} \langle I_1 | H | I_2 \rangle}{\sum_{I'} |c_{I'}|^2} . \quad (14)$$

In order to treat this model variationally we now employ a Jastrow Ansatz, given by

$$c_I = (-1)^{\phi(I)} \langle I | \prod_{i < j} \left[ 1 + f(i, j) (P_i^\uparrow P_j^\downarrow + P_i^\downarrow P_j^\uparrow) \right] | I \rangle \quad (15)$$

where the  $P^\uparrow$  and  $P^\downarrow$  are the usual projection operators of the spin-half ‘up’ and ‘down’ states respectively. The simplest approximation is to set the value of  $f(i, j)$  to be  $f_1$  (a scalar variable) if  $i$  and  $j$  are nearest neighbors, and to be zero otherwise. The expectation value of Eq. (14) may now be evaluated directly, although we explicitly restrict the sums over all states in Eq. (14) to those states in which  $m(I)$  is an even number in order to reflect the symmetries of the Hamiltonian [8]. The variational ground-state energy is minimized with respect to  $f_1$  at each value of  $\Delta$ , and the different sign rules for this system are utilized in separate calculations. We find that the best results for this variational Ansatz (for chains of length  $N \leq 16$ ) are those which utilize the correct sign rule in each regime, and Fig. 1 illustrates these results compared to those of an exact diagonalization calculation for a chain of length  $N = 12$ . (The accuracy of the variational calculations with  $N = 12$  compared to extrapolation in the limit  $N \rightarrow \infty$  via Padé approximants is estimated to be within about 4% for all  $\Delta$ .)

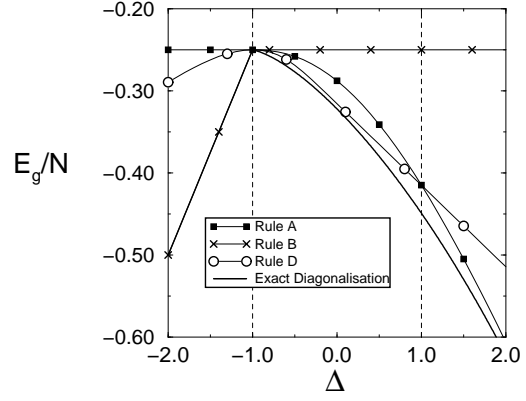


FIG. 1. Results for the ground-state energy of an anisotropic spin-half quantum spin chain (described in text) of length  $N = 12$ . The variational calculation utilizes the Jastrow Ansatz of Eq. (15) in which the sign rules (A), (B), and (D) are used in separate calculations and these results are compared to those of an exact diagonalization of this system.

This result is clearly true for any case in which one can prove an exact sign rule (e.g., those defined by Eqs. (3) and (10)) for a given model because any other choice would always contribute at least one non-zero positive contribution to the expectation energy from one of the ‘off-diagonal’ contributions (i.e.,  $I_1 \neq I_2$ ) in Eq. (14). We may therefore infer that the best possible variational Ansatz for a given model must always utilize the correct sign rule in the correct regime. However, a direct evaluation of the sums in Eq. (14) scales exponentially with increasing lattice size  $N$ , and so one must evaluate these summations using Monte Carlo (MC) techniques. In order to explain how this is achieved, we define a *probability distribution* for the Ising states  $\{|I\rangle\}$ , given by

$$P(I) = \frac{|c_I|^2}{\sum_{I'} |c_{I'}|^2} , \quad (16)$$

and the *local energy* of these states, given by

$$E_L(I) = \sum_{I_1} \frac{c_{I_1}}{c_I} \langle I | H | I_1 \rangle . \quad (17)$$

Equation (14) may be equivalently written as,

$$E = \sum_I P(I) E_L(I) , \quad (18)$$

where the sums over  $I_1$  in Eq. (17) and  $I$  in Eq. (18) run over all, or possibly some symmetry-constrained subset (e.g., the subset of Ising basis states  $|I\rangle$  for which  $m(I)$  is even), of the full set of Ising basis states. The MC procedure approximates the summation over  $I$  by performing a directed random walk with respect to  $|I\rangle$  based on the probability distribution  $P(I)$ . At each point of the MC ‘summation’ procedure one ‘steps’ from one state  $|I\rangle$  to another  $|I'\rangle$  (where  $|I'\rangle$  is one of a number of states accessible to  $|I\rangle$  via the off-diagonal elements of  $H$ ) with a

given probability which is dependent on  $P(I)$  and  $P(I')$ . Hence, it is possible to ‘cover’ all possible Ising states given enough run-time, although one samples the most important states the most often. Hence, in this manner an accurate approximation (to within statistical error) to the sum in Eq. (18) is built up. Also, the exponentially increasing problem with lattice size  $N$  is reduced to a problem that scales linearly with both  $N$  and the number of MC moves in a particular run. Hence, systems of larger lattice size may be treated.

We note, however, that the sign rule *does not* affect the random walk which simulates the summation over  $|I\rangle$  in Eq. (18) in such a variational MC calculation because the probability distribution of Eq. (16) is proportional to  $|c_I|^2$ . By contrast, we may see from the expression for the local energy of Eq. (17) that each and every ‘off-diagonal’ contribution (i.e.,  $I \neq I_1$ ) to the local energy can only be ensured *always* to be negative when the correct sign rule in the correct regime is used. The average variational ground-state energy, evaluated using the MC procedure outlined above, is the average of the local energies throughout the lifetime of the run. Hence the average variational MC ground-state energy can only ever be ensured to be lowest (to within statistical error) when the correct sign rule is utilized within the variational Ansatz (e.g., in the Jastrow Ansatz of Eq. (15)).

Let us finally turn our attention from variational MC estimates to full stochastic simulations of finite lattices by QMC techniques. All QMC methods at zero temperature basically project the exact ground state  $|\Psi\rangle$  of a given many-body Hamiltonian  $H$  out of an initial trial state  $|\Phi\rangle$  not orthogonal to  $|\Psi\rangle$ , by repeated applications of some suitable projection operator,  $G = G(H)$ . This operation can be formally expressed as a path integral over many-particle trajectories in configuration space. Furthermore, it can thus be represented by a stochastic process, which may itself be simulated computationally by the random walks of a sampled set of independent “walkers” through the configuration space. The main limitation to the applicability of such QMC techniques arises from the positivity requirement,

$$p(c, c') \equiv \langle c | G | c' \rangle \frac{\Phi(c')}{\Phi(c)} > 0, \quad (19)$$

on the probability  $p(c, c')$  for a walker to make a transition from an initial configuration  $|c\rangle$  to another configuration  $|c'\rangle$  along a random walk, where  $\Phi(c)$  is the wave function of the initial trial state.

For fermionic systems, the minus sign problem associated with  $p(c, c')$  ensures that QMC calculations are much more difficult than for bosons. Thus, the computer time for bosonic simulations to give results of a specified accuracy scales algebraically with (i.e., as some positive power of) the system size,  $N$ . By contrast, when the wave function being sampled is not positive-definite, and

hence cannot itself be regarded as a probability distribution, no “exact” simulation method has been discovered that does not scale exponentially with  $N$ . Without some prior knowledge of the nodal surface a QMC simulation will always eventually relax to the corresponding bosonic wave function. For the typical spin-lattice problem for which no such exact knowledge is available most QMC attempts to alleviate the minus sign problem, such as transient estimation, are infeasible due to its severity. In these cases a recently proposed lattice variant [9] of the fixed-node QMC (FNQMC) method [10] seems to provide the only practicable QMC-based approach.

Generally, results of FNQMC calculations are exact, within statistical errors limited solely by available computing power, only when the nodal surfaces of both the trial and exact ground-state wave functions coincide. Otherwise they yield variational upper bounds for the energy. On the other hand, other ground-state quantities such as the (magnetization or) staggered magnetization may be poorly estimated even when the energy is well estimated. How errors in the nodal surface affect such quantities is not well understood. In principle, however, their effects can be large. In this context the importance of such sign rules as those presented here becomes clear, in that they permit a complete circumvention of the QMC minus sign problem. Indeed, it remains an open and challenging problem as to whether such complete or even partial sign rules can be found for other highly correlated lattice systems which also suffer from the minus sign problem. Of particular interest, for example, would be to attempt to extend our work to both electron-lattice models and frustrated spin-lattice models.

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- [1] W. Marshall, 1955, *Proc. Roy. Soc. A*, **232**, 48 (1955).
  - [2] E.H. Lieb and D.C. Mattis, *J. Math. Phys.* **3**, 749 (1962).
  - [3] E.H. Lieb, T.D. Schultz, and D.C. Mattis, *Ann. Phys.* **16**, 407 (1961).
  - [4] O. Perron, *Math. Ann.* **64**, 248 (1907); G. Frobenius, *Sitzungsber. Preuss. Akad. Wiss. (Berlin)*, 471 (1908); R.A. Horn and C.R. Johnson, “Matrix Analysis,” (Cambridge University Press, Cambridge, 1985).
  - [5] R.G. Munro, *Phys. Rev. B* **13**, 4875 (1976).
  - [6] J.B. Parkinson, *J. Phys. C: Solid State Phys.* **10**, 1735 (1977).
  - [7] D.J. Klein, *J. Chem. Phys.* **77**, 3098 (1982).
  - [8] R.F. Bishop, D.J.J. Farnell, J.B. Parkinson, *J. Phys.: Condens. Matter* **8**, 11153 (1996).
  - [9] D.F.B. ten Haaf, H.J.M. van Benmel, J.M.J. van Leeuwen, W. van Saarloos, and D.M. Ceperley, *Phys. Rev. B* **51**, 13039 (1995).
  - [10] D.M. Ceperley and B.J. Alder, *Phys. Rev. Lett.* **45**, 566 (1980).